

# Luttinger Sum Rule in Slave-Particle Theories

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(Dated: 7 November 2002)

The long-standing belief is that the mean-field-like decoupling procedures applied to the slave-particle representations of the problems with strong local interaction violate Luttinger sum rule. The number of occupied resonant states is small and typically equal to the deviation from the sum rule, shedding doubt on the overall results. It is therefore illustrated, on the example of the Emery model for the high- $T_c$  superconductors, that, through the consistent application of the mean-field procedure to the Hamiltonian and the propagators, the sum rule is restored and the resonant band conserved. In addition to the resonant band, the electron spectrum contains large number of occupied states at the bare site-energy of the ion with strong repulsion. These results can be straightforwardly generalized to the other similar problems.

PACS numbers: 71.10.Fd, 71.27.+a

Keywords: strongly correlated systems, slave-boson method, Luttinger sum rule

The study of strongly correlated electron systems has been one of the most active research fields of solid state physics for a long time. In the present context, it is appropriate to mention Friedel/Anderson and Kondo impurity problems, including the case of Kondo lattice, the (extended) Hubbard models and their t-J derivatives and the Emery model of the  $\text{CuO}_2$  conducting planes for the high- $T_c$  rare-earth oxides with its t-J limit. General feature of these models is the appearance of the resonant state, or the resonant band in the translationally invariant case, on the top of a large fermionic background.

Many methods used in the treatment of strongly correlated systems introduce auxiliary fermions and bosons [1, 2, 3, 4, 5]. Although the transformation to new particles is exact at the outset, it actually becomes useful in approximations applied to the coupled fermion-boson system. Especially simple situation occurs when only the on-site interaction is retained and taken to infinity, because then only one fermion and one boson field are sufficient. These two fields are coupled and various decoupling schemes, such as mean-field approximations with their Gaussian extensions or the local gauge theories where the vertex corrections are ignored, lead to representation of the Green function of the physical electron as the product (or convolution) of the auxiliary fermion and boson Green functions. This results in (satisfactory) appearance of the resonant state or band. However, as the rule, the weight of the resonance is small and of the order of the error in the Luttinger sum rule associated with the calculation of the resonance [6, 7, 8]. This sheds doubt on the ability of the simple decoupling schemes to describe the resonant band, its weight being of the order of the error.

The improvements were attempted by including the fermion-boson interactions in high orders with vertex corrections ignored, considering in particular the non-local

string fields, with the conclusion that the Luttinger sum rule cannot be restored [7]. Alternatively, the time dependence of the boson fields was postulated unimportant in the calculation of the physical particle propagation [9]. This restores the Luttinger sum rule, but results in the appearance of the unphysical incoherent background in the wide energy range of the spectral density.

A simple argument is hence given that calculating the physical particle propagator consistently with the overall decoupling procedure the Luttinger sum rule is recovered without eliminating the resonant band. The large spectral background appears, but localized in energy to the vicinity of the non-renormalized deep level. To be specific, the reasoning is illustrated on the case of the 2d Emery model in the slave-boson representation [10, 11, 12, 13, 14, 15], treated in the mean-field approximation, but the reasoning can be straightforwardly extended to the other models in similar decoupling schemes.

In the usual definition of the Emery model [16] for the  $\text{CuO}_2$  plane where  $\varepsilon_d$  and  $\varepsilon_p$  are the bare Cu and O site energies respectively,  $t_0$  is the bare Cu-O hopping,  $t'$  is the O-O hopping and  $U_d$  is the Cu on-site Coulomb repulsion. When  $U_d \approx \infty$  double occupancy is forbidden and the original fermion field  $c_R$  (spin indices are not shown for brevity) which annihilates the d-hole on the Cu site is expressed in term of boson  $b_R$  and fermion  $f_R$  as

$$c_R = f_R b_R^\dagger \quad (1)$$

and  $c_R^\dagger$  is given as its conjugate.

The Hilbert space associated with auxiliary fermions and bosons is highly redundant, and the physical subspace is characterized by the no-double occupancy condition

$$Q_R = f_R^\dagger f_R + b_R^\dagger b_R = 1. \quad (2)$$

Using Eq.(1) for copper sites, combined with the fermion fields  $p_R$  associated with oxygen sites, the Emery

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Hamiltonian transforms to

$$H = \sum_{s,R} [\varepsilon_d n_R^d + \varepsilon_p \sum_{i=x,y} n_{R,i}^p + \sum_{i=x,y} t_0 (f_R^\dagger b_{R,i} p_{R,i} + \sum_{\delta} f_R^\dagger b_{R+\delta,i} + h.c.) + t' (p_{R,x} p_{R,y} + h.c.)], \quad (3)$$

where  $R$  is a site index and  $\delta$  denotes nearest neighbors. Total number  $N$  of  $d$  and  $p$  fermions transforms analogously to  $H$  of Eq.(3). The representations of  $N$  and  $H$  are however not unique, as any operator equal to zero in  $Q_R = 1$  subspace, such as  $\nu f_R^\dagger f_R b_R^\dagger b_R$ ,  $\nu$  arbitrary constant, can be added to  $n_R^d$ . In other words,  $n_R^d$  can be represented as

$$n_R^d = n_R^f (b_R b_R^\dagger + \nu b_R^\dagger b_R), \quad (4)$$

the expression in the brackets equal to one in  $Q_R = 1$  space. Irrelevant in the exact calculations, the choice of  $\nu$  in the brackets becomes important for any approximate procedure not confined to the  $Q_R = 1$  space. Then the only way to keep  $n_R^d$  in  $N$  and  $H$  independent on the boson variables, as it is in the exact calculations, is to choose

$$\nu = -1 \quad (5)$$

in Eq.(4).

Noteworthy,  $Q_R$  commutes with  $H$  and  $N$  and therefore they are diagonalized in the  $Q_R = 1$  subspace. In particular, the physical ground state  $|G\rangle$  is the state of the lowest energy in that subspace. The mean-field slave-boson procedure (MFSB) approximates  $|G\rangle$  by the product of the ground state  $|G(b_0)\rangle$  of the displaced harmonic oscillator  $b' = b - b_0$  and the ground state of the  $n = 1 + x$  free  $f$ -fermions  $|G_0(f)\rangle$

$$|G\rangle \approx |G_{MF}\rangle = |G(b_0)\rangle \times |G_0(f)\rangle. \quad (6)$$

$|G(b_0)\rangle$  has the property that  $\langle b_R^\dagger b_R \rangle = \langle b_R^\dagger \rangle^2 = \langle b_R \rangle^2 = b_0^2$ .  $|G_{MF}\rangle$  has a component outside the  $Q_R = 1$  subspace, which is minimized with the requirement that  $Q_R = 1$  is satisfied at average

$$\langle G_{MF} | Q_R | G_{MF} \rangle = \langle n^f \rangle + b_0^2 = 1, \quad (7)$$

using Eq.(2). Even when  $|G_{MF}\rangle$  is chosen to satisfy Eq.(7), its component outside  $Q_R = 1$  subspace is still present. This can be easily seen from the calculation of  $\langle n_d \rangle$  using Eq.(4),  $\langle n_R^d \rangle = \langle n_R^f \rangle (1 + (\nu + 1)b_0^2)$ . From this result, it is obvious that, in the presence of long-range order  $b_0 \neq 0$ , the use of  $|G_{MF}\rangle$  should be combined with the choice  $\nu = -1$  in Eq.(4) leading the equality

$$\langle n_R^d \rangle = \langle n_R^f \rangle. \quad (8)$$

Using further Eq.(6), boson field can be averaged out from  $H + \lambda \sum Q_R$  of Eqs.(3) and (2). Eq.(8), i.e. Eq.(5) is essential in evaluating the local term. The result is the

MF fermion Hamiltonian which describes free  $f$ -fermions on the  $CuO_2$  lattice with the effective (renormalized) parameters of the non-interacting Emery model  $t = b_0 t_0$  and  $\varepsilon_f = \varepsilon_d + \lambda$ , while  $t'$  remains unchanged. On the other hand, when the fermion variables are averaged out, the Hamiltonian  $\lambda b_R'^\dagger b_R'$  of the displaced  $b_R'$  harmonic oscillator is obtained. Here again, the choice  $\nu = -1$  is important because it eliminates the  $b'$  dependence from the local term of  $H + \lambda \sum Q_R$ , i.e. it leaves  $\lambda$  to govern alone the energy of  $b'$  boson.

Noting that the energy of the  $b'$  boson field vanishes for  $|G(b_0)\rangle$ ,  $t$  (i.e.  $b_0$ ) and  $\lambda$  are found by minimizing the ground state energy  $E_0$  of the fermion MF Hamiltonian at fixed number of fermions  $n = 1 + x$ .

Time-dependent Gaussian fluctuations around MF saddle point are considered in the next step. A quantity convenient to discuss for such a purpose is the single particle propagator between the Cu sites. According to Eq.(1)

$$G_{RR'}^d(\tau) = (-i) \langle G | T f_R^\dagger(\tau) b_R(\tau) f_{R'} b_{R'}^\dagger | G \rangle. \quad (9)$$

As in the case of  $n_d$  in Eq.(4), the choice of operators entering the autocorrelation function  $G_{RR}$  in Eq.(9) is not unique, because in particular  $\nu f_R^\dagger f_R b_R^\dagger b_R$  can be added to it without changing  $G_{RR}^d$

$$G_{RR}^d(\tau) = (-i) b_0^2 \langle G | T f_R^\dagger(\tau) f_R b_R(\tau) b_R^\dagger + \nu f_R^\dagger f_R b_R^\dagger b_R | G \rangle. \quad (10)$$

The  $f$ -fermions and  $b'$ -bosons decouple, when the  $f$   $b'$  coupling is omitted in the MF approximation, i.e.  $G^d$  decouples into the product of fermion and boson propagators. Noting that to this order the  $b'$  boson propagator is local

$$iG_{RR'}^d(\tau) = b_0^2 \langle G_0(f) | T f_R^\dagger(\tau) f_{R'} | G_0(f) \rangle, \quad R \neq R', \quad (11)$$

and

$$iG_{RR}^d(\tau) = \langle G_0(f) | T f_R^\dagger(\tau) f_R | G_0(f) \rangle \langle G(b_0) | T b_R(\tau) b_R^\dagger | G(b_0) \rangle + \nu \langle n^f \rangle b_0^2, \quad (12)$$

where  $\nu$  is kept explicit in order to follow its trace in the following discussion. Note that the operator in Eq.(10) reduces to  $n^d$  of Eq.(4) at  $\tau = 0$ . Consistently with the MF choice  $\nu = -1$ , Eq.(5) of the MF procedure, this choice should be repeated in Eq.(12) when  $|G\rangle$  is replaced by  $|G_{MF}\rangle$  in order to satisfy sum rule  $\langle n^d \rangle = \langle n^f \rangle$  of Eq.(8). General structure  $\eta^2 - \bar{\eta}^2$  of Eq.(12) is then obtained for the correlation function  $G_{RR}$  when long-time/long-range order ( $b_0 \neq 0$ ) is present. This structure justifies the time-independent choice of the  $\nu$ -operator in Eq.(10).

Mean-field free-particle propagators appear in Eqs.(11) and (12). The Fourier transform ( $R = R'$  included) of the MF  $\nu = -1$  free-fermion propagator is

$$G^f(\omega, \mathbf{k}) = \frac{|m_f(\mathbf{k})|^2}{\omega - \varepsilon(\mathbf{k}) + i\eta \text{sign}(\varepsilon(\mathbf{k}) - \mu)}, \quad (13)$$

where  $\varepsilon(\mathbf{k})$  is the dispersion of the free f-fermion band and  $|m_f(\mathbf{k})|^2$  is the probability of finding it on the Cu-site, both quantities obtained by MFSB. MF  $\nu = -1$  boson propagator  $\langle G(b_0) | T b'(\tau) b'^{\dagger} | G(b_0) \rangle$  in Eq.(12) is given by

$$D^{b'}(\omega) = \frac{1}{\omega - \lambda + i\eta} \quad (14)$$

because, as already mentioned, free dynamics of the boson  $b'$  is local and determined at  $\nu = -1$  by the frequency  $\lambda$  (Cartesian gauge of the boson field is meant here). Combining Eqs.(12), (13) and (14),  $G_{RR}^d(\omega)$  reads

$$G_{RR}^d(\omega) = \int \frac{d\mathbf{k}}{(2\pi)^2} \theta(\mu - \varepsilon(\mathbf{k})) \frac{|m_f(\mathbf{k})|^2}{\omega - (\varepsilon(\mathbf{k}) - \lambda) - i\eta} + [G_{RR}^f(\omega) - i\pi\nu\langle n_f \rangle \delta(\omega)] b_0^2 \quad (15)$$

The first term in Eq.(15) describes [8] the local excitation of the dispersionless level of the energy  $\varepsilon_d = \varepsilon_f - \lambda$ . The number of states associated with this level is given by the integration of  $\pi^{-1} \text{Im} G^d(\omega)$  over frequency, and, as it can be easily seen using Eq.(15), it is equal to  $\langle n^f \rangle$ . The excitation energy  $\Delta_{pd} = \varepsilon_p - \varepsilon_d$  of the dispersionless level at  $\varepsilon_d$ , large when  $\lambda$  is large, is observed in the high-energy spectroscopies.

The second term in Eq.(15) together with Eq.(11) forms nearly half-filled resonant band described by  $b_0^2 G^f(\omega, \mathbf{k})$ . Band-dispersion of the resonant band of the weight  $b_0^2$  is obviously the one of the MF solution [8]. The latter shows that the off-site dynamics is determined by the small energy scales:  $t < t_0$  (and  $t' < t_0$  in the spirit of the Emery model). These scales should be observed in low frequency spectroscopies, such as ARPES.

The integrated contribution of the second term in Eq.(15) to  $\pi^{-1} \text{Im} G^d(\omega)$  is  $b_0^2 \langle n^f \rangle$ . It corresponds to the contribution of the resonant band  $b_0^2 G^f(\mathbf{k}, \omega)$  to  $\langle n^d \rangle$ . Together with the contribution  $\langle n^f \rangle$  of the first term and  $\nu b_0^2 \langle n^f \rangle$  of the third, long-range order term it gives

$\langle n^d \rangle = \langle n^f \rangle (1 + (1 + \nu) b_0^2)$ , which for  $\nu = -1$  reproduces the Luttinger sum rule  $\langle n^d \rangle = \langle n^f \rangle$  of Eq.(8). In other words, the long-range contribution cancels exactly the contribution to  $\langle n^d \rangle$  of the resonant band, without removing the resonant band itself.

Unfortunately, numerous previous calculations for the Emery, Hubbard or Kondo problems [6, 7, 8, 9, 17] amount or are analogous to taking  $\nu = -1$  in the MF procedure when calculating the energy, but leaving [7, 8, 9]  $\nu = 0$  in Eqs.(10-15) for the propagators.  $\nu = 0$  leads to  $\langle n^d \rangle = \langle n^f \rangle (1 + b_0^2)$ , i.e. to the breakdown of the Luttinger sum rule Eq.(8), the discrepancy arising from the contribution of the resonant band. It is therefore important to point out that by simple inclusion of the long-range/long-time term in  $G_{RR}$ , by choosing  $\nu = -1$  in Eqs.(10) and (12), solves the problem of the sum rule without removing the resonant band.

Finally, it should be emphasized once again that the MF content of the above argument is not essential for the restoration of the Luttinger sum rule. The latter relies on two assumptions. The first is that the ground state can be decoupled [7] into the product of boson and fermion states, as in Eq.(6). The second assumption is that the long-time order is present in the autocorrelation function  $iG_{RR}$ , leading to the inclusion of the negative  $\nu = -1$  time-independent term into Eq.(12). The Hamiltonian has no explicit role in this argument, except that the correlation functions appearing in the calculation of the (ground state) energy have to be evaluated consistently with  $G$ . The present argument applies therefore to the entire class of Hamiltonians with large, local interactions [17], amenable to the slave-particle analysis.

## Acknowledgments

This work was supported by Croatian Ministry of Science under the project 119-204.

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